Numerical simulations of diffusion-limited aggregation on the torus

1988 J. Phys. A: Math. Gen. 21 L159

(http://iopscience.iop.org/0305-4470/21/3/008)

J. Phys. A: Math. Gen. **21** (1988) L159-164. Printed in the UK

LETTER TO THE EDITOR

Numerical simulations of diffusion-limited aggregation on the torus

M Wolf

Institute of Theoretical Physics, University of Wrocław, ul Cybulskiego 36, PL 50-205 Wrocław, Poland

Received 25 November 1987

Abstract. The results of numerical simulations of diffusion-limited aggregation on the torus are presented. The usual random walk was generalised by allowing the particle to perform jumps of length equal to s lattice spacings, $s \geq 1$. Patterns with periodic structure were obtained.

Recently there has been an increasing interest in the study of irreversible kinetic processes leading to the formation of fractal patterns. A simple stochastic model for the formation of clusters of particles in two-dimensional space was proposed by Witten and Sander (1981, 1983). In their model, called diffusion-limited aggregation (DLA), a single particle walks randomly on the square lattice until it reaches another particle ('seed'), located usually in the centre of the lattice. Next, a new particle initiates its random walk. If the particle contacts the cluster (now built of two particles) it is incorporated into the cluster and the cluster grows. This process is repeated many times and leads to ramified structures possessing remarkable scaling properties (see figure 1, where a cluster of 3000 particles is shown). For example, the number N of

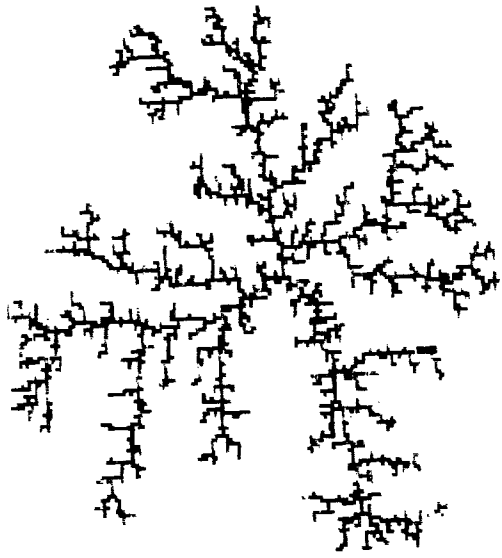

Figure 1. Typical aggregate obtained from 3000 particles by means of usual DLA on the torus.

0305-4470/88/030159+06$02.50

particles contained inside the circle of radius R grows as

$$N(R) \sim R^D \tag{1}$$

where $D \approx 1.7$ is the fractal dimension (Mandelbrot 1982). It is believed that the value 1.7 for D is universal, i.e. it does not depend on the lattice, which was confirmed for the triangular lattice by Witten and Sander (1981, 1983) and for the non-lattice case by Meakin (1983a).

Some modifications and different techniques for computer simulations have been discussed (for reviews see Sander (1985), Stanley and Ostrovsky (1986) and Herrmann (1986)). Variants of the original DLA include the introduction of the probability distribution for the sticking of particles (Meakin 1983a), superimposition of the drift on the diffusion (Meakin 1983b), using so-called Levy flight instead of the usual diffusion (Meakin 1984), modification of the sticking rule (Kertész and Vicsek 1986), and so on. Also, electric breakdowns in dielectrics lead to fractal structures for the discharge patterns (Niemeyer *et al* 1984). Some different algorithms for computer simulations have also been used (see, e.g., Meakin (1983a) and Ball and Brady (1985)). The aim of these modifications was the reduction of the duration of computer simulations. For example, in Meakin's (1983a) simulations a particle was killed if it went sufficiently far away from the cluster and the new particle started on the circle surrounding the aggregate. To our knowledge, there is still no satisfactory theory of DLA (see, however, Gould *et al* (1983), Muthukumar (1983) and Halsey *et al* (1986)).

In this letter we shall present preliminary results of the computer simulation of DLA on the torus. The recipe for the formation of aggregates was the following. Let us imagine the square lattice with L sites along one edge. One of the edges was chosen with probability $\frac{1}{4}$ and on it the starting point for the random walk was chosen with probability $1/L$. We generalised the usual random walk by allowing the particle to perform jumps of length equal to s lattice spacings, $s \geq 1$, with probability $\frac{1}{4}$ in one of four directions: up, down, left and right. We imposed on the random walk the periodic boundary condition that a particle crossing one of the edges appears on the opposite side (so the number of bonds between sites is also equal to L). In other words, the particle performs a random walk on the torus. As we took the number L to be prime (see below) it was possible to locate the seed in the centre of the square. The sticking rule was the usual one, i.e. the particle was incorporated into the aggregate on the first contact with it, providing that one particle only can occupy each site. (For $s = 1$, i.e. for usual DLA, it is impossible that the walker will fall into the site already occupied.) We should add that we allowed the particle to walk on the sites already occupied, i.e. on the aggregate.

For the termination of the aggregation process, the trajectory of each particle should reach the cluster. In other words, the trajectory should fill out the whole torus. It is obvious that for usual diffusion with $s = 1$ each site can be reached by the walker. But in a case of the random walk with length of step $s > 1$, the trajectory will fill out the torus only when L and s are mutually prime, i.e. when the greatest common divisor (GCD) of L and s is equal to 1. It is common to denote the GCD of two natural numbers a and b by (a, b), so for the 'ergodicity' of the random walk the following condition should be satisfied:

$$(L, s) = 1. \tag{2}$$

The above condition can be justified in the following way. Using the following identity:

$$(A \bmod C + B) \bmod C = (A + B) \bmod C$$

the x coordinate, for example, of the particle after some number of jumps can be written as

$$x = (x_0 + ks) \bmod L = x_0 + ks - L[(x_0 + ks)/L] \qquad k \in \mathbb{Z}$$

where $[r]$ denotes the integer part of the number r and x_0 is a starting point. Denoting $q = [(x_0 + ks)/L]$ and shifting $x - x_0 \to x$ we can write

$$x = ks - Lq.$$

The trajectory of the random walk will fill out the torus if and only if the above equation has integer solutions k and q for each x. From the theory of Diophantine equations (e.g. Courant and Robbins 1961) it is known that the equation

$$ax + by = c$$

has integer solutions for x and y if and only if c is a multiple of (a, b). The only way to fulfil the requirement that each x should be a multiple of (L, s) is the condition (2). The easiest and most convenient way to conform to (2) is to take L prime. In a case when $(L, s) \neq 1$ the particle will be moving on the sublattice with period (L, s) because only coordinates divisible by (L, s) can be visited by a walker.

Due to our modest computer abilities we were able to make aggregates of up to 6000 particles on a lattice of 173×173 sites, so the ratio of filled pixels to all pixels was equal to 0.2005 .... We used the following random number generator:

$$Z_{i+1} = AZ_i \bmod C \qquad A = 1203\,248\,318, \qquad C = 2^{31} - 1$$

which is claimed to possess weak correlations (Fishman and Moore 1982). Figure 2 presents aggregates obtained by numerical simulations with different lengths of step. This figure shows that typical shapes of three kinds are produced for $s > 1$. (Figure 1 was made using the same program but for $s = 1$ to check the correctness of it.) In all cases periodic structures in the outer regions (resembling crystals) were obtained. We see that for small steps (see figure 2(a) for $s = 3$) the aggregates have peninsulas and gulfs, but for larger steps of random walk more regular objects are formed. We found that the fractal dimension measured via equation (1) is not a good characterisation of aggregates obtained for $s > 1$ because the slope of the log N against log R plot is not a constant but either decreases slowly with R (for small s) or oscillates with period equal to the period of the 'crystallic' lattice produced (for larger s, such as $s = 29$, figure 2(d)). Nevertheless, it should be mentioned that the slope of the log N against log R plot varies between 1.8 and 1.5. It seems that there is another quantity needed to distinguish qualitatively the patterns in figures 1 and 2. It could be expected that for $s > 1$ the particles would be able to penetrate deeper into the aggregate than for usual DLA, but this is not so, as can be seen from figure 3 where the last 3000 particles are plotted. We would like also to mention that the patterns shown in figures 2(a)-(c) visually resemble the ones obtained in another way by Sawada *et al* (1982) (see figure 2 in their paper) and it seems that there should be a connection between their control parameter called the tip priority factor and our length of steps. Let us add that these authors found it necessary to introduce two fractal dimensions to characterise their patterns, because the slope of the plot of log N against log R was not constant for all R.

Finally let us add a few 'phenomenological' remarks. First of all, it should be stressed that the characteristic quasiperiodic patterns of aggregates are intimately connected with the fact that all particles started from the same boundary. For example,

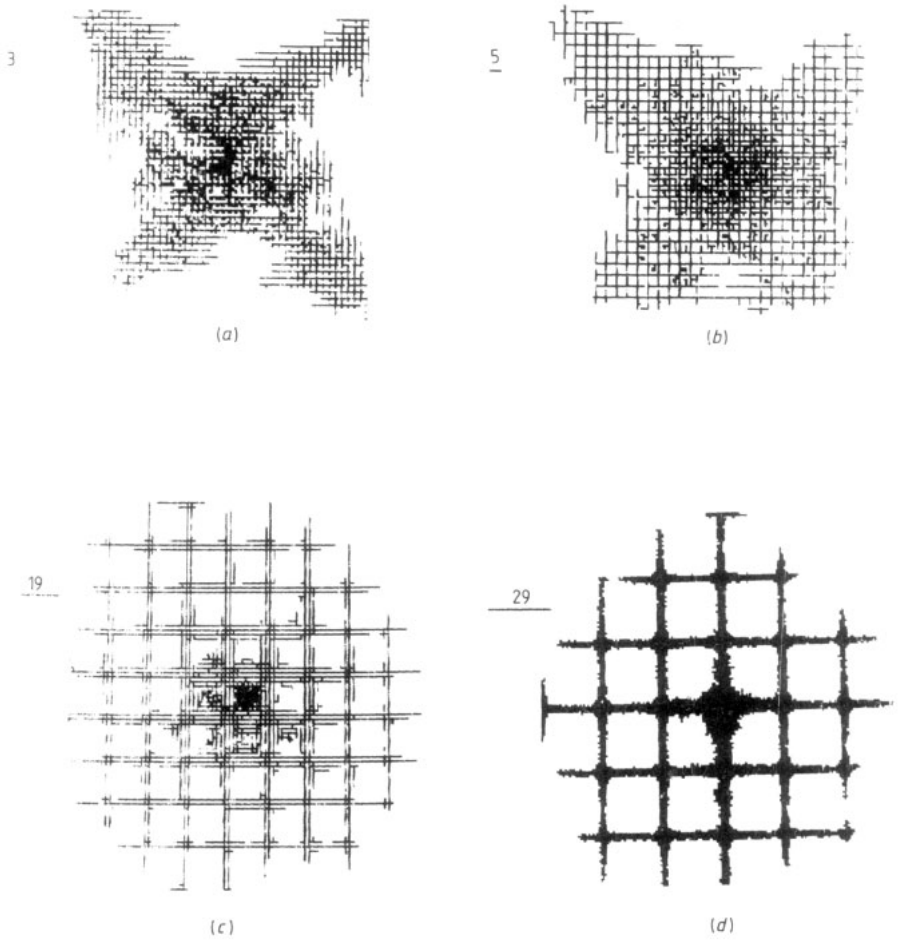

Figure 2. Typical aggregates obtained by means of DLA on the torus with length of step $s =$ (*a*) 3, (*b*) 5, (*c*) 19 and (*d*) 29. The step is drawn in the upper left-hand corner of each figure. The number of particles is equal to 6000 in each case.

when for $s = 19$ we chose the starting points from the four strips of width equal to s, we did not obtain the strange object seen in figure 2(*c*) but the circle densely filled with particles. Secondly, for the random walk with $s > 1$ the sites lying on the straight lines x, $y = ks$, $k \in \mathbb{Z}$, are visited earlier by the walker than other ones. This fact explains the quasiperiodicity of the aggregates. We are now trying to formalise these observations.

I would like to thank Professor L Turko for reading the manuscript. I also wish to thank Drs A Huczyński and A Kozek for providing me with a procedure for generating random numbers.

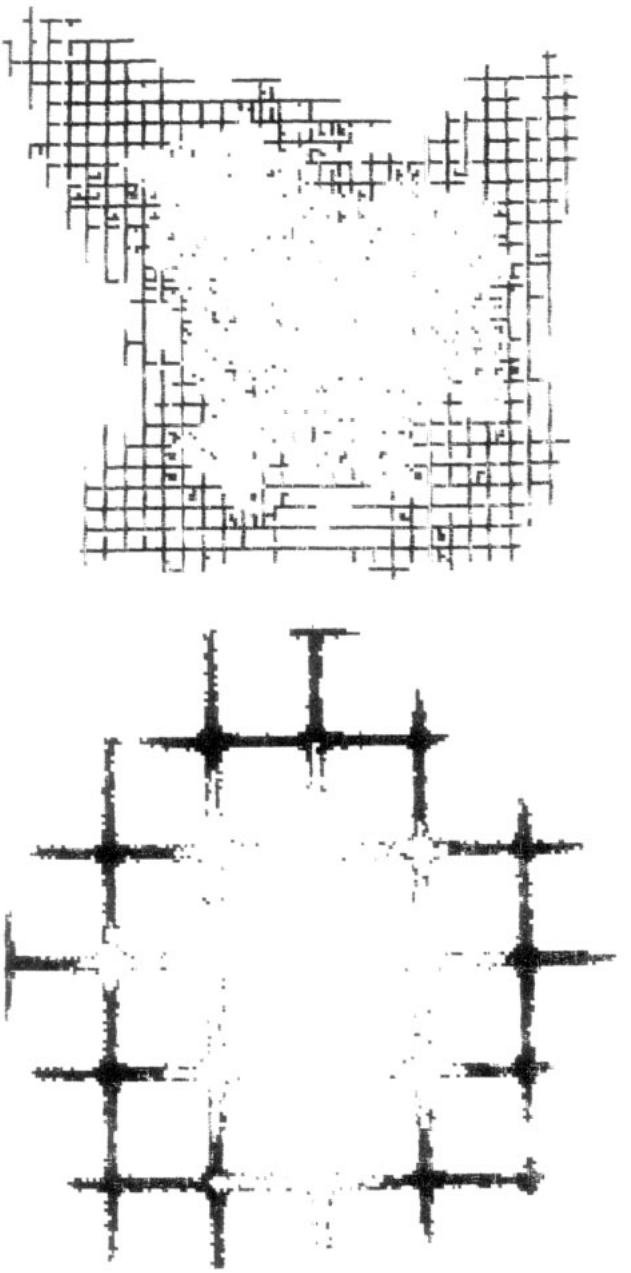

Figure 3. The last 3000 particles which hit the aggregate plotted for the aggregates from figure 2(*b*) in the upper part and from figure 2(*d*) in the lower part. It is seen in the lower part that in spite of the large length of step ($s = 29$) the particles do not penetrate deeply into the aggregate.

References

Ball R C and Brady R M 1985 *J. Phys. A: Math. Gen.* **18** L809
Courant R and Robbins H 1961 *What is Mathematics?* (Oxford: Oxford University Press)
Fishman G S and Moore L R 1982 *J. Am. Stat. Assoc.* **77** 129
Gould H, Family F and Stanley H E 1983 *Phys. Rev. Lett.* **50** 686
Halsey T C, Meakin P and Procaccia I 1986 *Phys. Rev. Lett.* **56** 854
Herrmann H J 1986 *Phys. Rep.* **136** 153
Kertész J and Vicsek T 1986 *J. Phys. A: Math. Gen.* **19** L257
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
Meakin P 1983a *Phys. Rev.* A **27** 1495
—— 1983b *Phys. Rev.* B **28** 5221
—— 1984 *Phys. Rev.* B **29** 3722
Muthukumar M 1983 *Phys. Rev. Lett.* **50** 839
Niemeyer L, Pietronero L and Wiesmann H J 1984 *Phys. Rev. Lett.* **52** 1033
Sander L 1985 *Scaling Phenomena in Disordered Systems* ed R Pynn and A Skjeltorp (New York: Plenum) p 31
Sawada Y, Ohta Y, Yamazaki M and Honjo H 1982 *Phys. Rev.* A **27** 3557
Stanley H E and Ostrovsky N (ed) 1986 *On Growth and Form* (Dordrecht: Martinus Nijhoff)
Witten T and Sander L 1981 *Phys. Rev. Lett.* **47** 1400
—— 1983 *Phys. Rev.* B **27** 5686